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stn


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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  JUL 28  CA/CAplus patent coverage enhanced
 NEWS  3  JUL 28  EPFULL enhanced with additional legal status
                  information from the epoline Register
 NEWS  4  JUL 28  IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
 NEWS  5  JUL 28  STN Viewer performance improved
 NEWS  6  AUG 01  INPADOCDB and INPAFAMDB coverage enhanced
 NEWS  7  AUG 13  CA/CAplus enhanced with printed Chemical Abstracts
                  page images from 1967-1998
 NEWS  8  AUG 15  CAOLD to be discontinued on December 31, 2008
 NEWS  9  AUG 15  CAplus currency for Korean patents enhanced
 NEWS 10  AUG 27  CAS definition of basic patents expanded to ensure
                  comprehensive access to substance and sequence
                  information
 NEWS 11  SEP 18  Support for STN Express, Versions 6.01 and earlier,
                  to be discontinued
 NEWS 12  SEP 25  CA/CAplus current-awareness alert options enhanced
                  to accommodate supplemental CAS indexing of
                  exemplified prophetic substances
 NEWS 13  SEP 26  WPIDS, WPINDEX, and WPIX coverage of Chinese and
                  and Korean patents enhanced
 NEWS 14  SEP 29  IFICLS enhanced with new super search field
 NEWS 15  SEP 29  EMBASE and EMBAL enhanced with new search and
                  display fields
 NEWS 16  SEP 30  CAS patent coverage enhanced to include exemplified
                  prophetic substances identified in new Japanese-
                  language patents
 NEWS 17  OCT 07  EPFULL enhanced with full implementation of EPC2000
 NEWS 18  OCT 07  Multiple databases enhanced for more flexible patent
                  number searching
 NEWS 19  OCT 22  Current-awareness alert (SDI) setup and editing
                  enhanced
 NEWS 20  OCT 22  WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                  Applications
 NEWS 21  OCT 24  CHEMLIST enhanced with intermediate list of
                  pre-registered REACH substances

 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.



Updated Search
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 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008

=> file reg
COST IN U.S. DOLLARS                                 SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                      0.21       0.21

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STRUCTURE FILE UPDATES:   24 OCT 2008  HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES:  24 OCT 2008  HIGHEST RN 1065816-63-8

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http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\577.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR



Updated Search
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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 00:33:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        2 TO ITERATE

100.0% PROCESSED        2 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             2 TO      124
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:34:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       37 TO ITERATE

100.0% PROCESSED       37 ITERATIONS                                14 ANSWERS
SEARCH TIME: 00.00.01

L3           14 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   181.12     181.33

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FILE COVERS 1907 - 27 Oct 2008  VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008  (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.



Updated Search
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stn


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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l3
L4            3 L3

=> s l4 and lim, z?/au
             41 LIM, Z?/AU
L5            1 L4 AND LIM, Z?/AU

=> d l5, ibib abs hitstr, 1

L5   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2005:395258  HCAPLUS
DOCUMENT NUMBER:          142:446921
TITLE:                    A preparation of acylurea- and sulfonylurea-connected
                          hydroxamates, useful as histone deacetylase (HDAC)
                          inhibitors
INVENTOR(S):              Lim, Ze-Yi; Wang, Haishan; Zhou, Yan
PATENT ASSIGNEE(S):       Sbio Pte. Ltd., Singapore
SOURCE:                   PCT Int. Appl., 145 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
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     WO 2005040101          A1    20050506    WO 2004-SG353            20041026
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     AU 2004284030          A1    20050506    AU 2004-284030           20041026
     CA 2543570             A1    20050506    CA 2004-2543570          20041026
     EP 1685094             A1    20060802    EP 2004-775672           20041026
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     JP 2007509930          T     20070419    JP 2006-537946           20041026
     MX 2006PA04735         A     20061214    MX 2006-PA4735           20060427
     US 20080070954         A1    20080320    US 2007-577462           20070927
PRIORITY APPLN. INFO.:                         US 2003-514013P     P    20031027
                                               WO 2004-SG353       W    20041026
OTHER SOURCE(S):          CASREACT 142:446921; MARPAT 142:446921
GI


Updated Search
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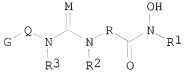

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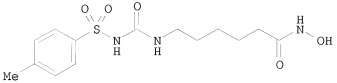


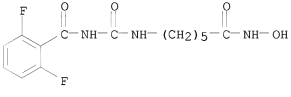
II

AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

IT 1044042-90-1 1044043-10-8
RL: PRPH (Prophetic)
(A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors)

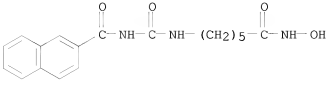
RN 1044042-90-1 HCAPLUS

CN Benzamide, 2,6-difluoro-N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX NAME)



RN 1044043-10-8 HCAPLUS

CN 2-Naphthalenecarboxamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX NAME)

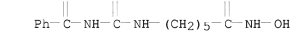


Updated Search

stn

IT 851365-34-9P 851365-36-1P 851365-37-2P
851365-41-8P 851365-43-0P 851365-45-2P
851365-46-3P 851365-48-5P 851365-49-6P
851365-50-9P 851365-70-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of acylurea- and sulfonylurea-connected hydroxamates useful as
HDAC enzyme inhibitors)

RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX
NAME)



RN 851365-36-1 HCAPLUS
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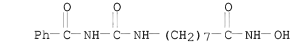

RN 851365-37-2 HCAPLUS
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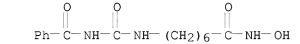

RN 851365-41-8 HCAPLUS
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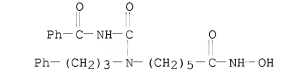
phenylpropyl)amino]carbonyl]- (CA INDEX NAME)



RN 851365-43-0 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]thioxomethyl]- (CA
INDEX NAME)

Updated Search

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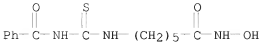
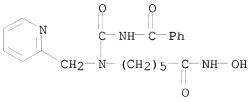


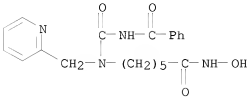
RN 851365-45-2 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](2-pyridinylmethyl)amino]carbonyl]- (CA INDEX NAME)



RN 851365-46-3 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](2-pyridinylmethyl)amino]carbonyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 851365-45-2
CMF C20 H24 N4 O4



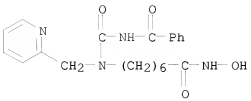
CM 2

CRN 76-05-1
CMF C2 H F3 O2

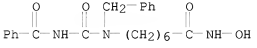
RN 851365-48-5 HCAPLUS
CN Benzamide, N-[[[7-(hydroxyamino)-7-oxoheptyl](2-pyridinylmethyl)amino]carbonyl]- (CA INDEX NAME)

Updated Search

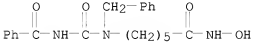
stn



RN 851365-49-6 HCAPLUS
CN Benzamide, N-[[[7-(hydroxyamino)-7-oxoheptyl](phenylmethyl)amino]carbonyl]-
(CA INDEX NAME)



RN 851365-50-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl](phenylmethyl)amino]carbonyl]-
(CA INDEX NAME)



RN 851365-70-3 HCAPLUS
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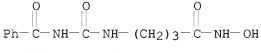
NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3

Updated Search

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stn


L5            1 S L4 AND LIM, Z?/AU

=> s l4 not l5
L6            2 L4 NOT L5

=> s l6 and wang, h?/au
         51308 WANG, H?/AU
L7            0 L6 AND WANG, H?/AU

=> s l6 and zhou, y?/au
         21640 ZHOU, Y?/AU
L8            0 L6 AND ZHOU, Y?/AU

=> d l6, ibib abs hitstr, 1-2

L6   ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:1447760  HCAPLUS
DOCUMENT NUMBER:          148:85678
TITLE:                    Solid oral dosage form containing deacetylase
                          inhibitor and an enhancer
INVENTOR(S):              Leonard, Thomas W.; O'Toole, Edel; Feeney, Orlagh
PATENT ASSIGNEE(S):       Merrion Research II Limited, Ire.
SOURCE:                   U.S. Pat. Appl. Publ., 38pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
     US 20070292512       A1    20071220    US 2007-761233          20070611
     WO 2007146234        A2    20071221    WO 2007-US13693         20070611
     WO 2007146234        A3    20080228
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              CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI,
              GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
              KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
              MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
              PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
              TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
          RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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              BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
              GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
              BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
PRIORITY APPLN. INFO.:                      US 2006-812523P     P  20060609
AB   The invention relates to a pharmaceutical composition, particularly oral dosage
     forms, comprising a DAC inhibitor in combination with an enhancer to
     promote absorption of the DAC inhibitor at the GIT cell lining.  The
     enhancer is a medium-chain fatty acid or derivative thereof having a carbon
     chain length of 6-20 carbon atoms.  In certain embodiments, the solid oral
     dosage form is a controlled-release dosage form such as a delayed-release
     dosage form.  Thus, a sustained-release tablet was prepared containing sodium
     caprylate 65.7%, heparin 13.3%, silica dioxide 0.5%, magnesium stearate
     0.5%, and mannitol 20.0%.



Updated Search
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IT 851365-34-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(solid oral dosage form containing deacetylase inhibitor and an enhancer)
RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX NAME)

L6 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:206787 HCAPLUS
DOCUMENT NUMBER: 146:287512
TITLE: Development and validation of high-performance liquid chromatography-tandem mass spectrometry assay for 6-(3-benzoyl-ureido)-hexanoic acid hydroxyamide, a novel HDAC inhibitor, in mouse plasma for pharmacokinetic studies
AUTHOR(S): Yeo, Pauline; Xin, Liu; Goh, Evelyn; New, Lee Sun; Zeng, Peizi; Wu, Xiaofeng; Venkatesh, P.; Kantharaj, Ethirajulu
CORPORATE SOURCE: Department of Pharmacokinetics and Drug Metabolism, SBIO Pte Ltd, Singapore, 117528, Singapore
SOURCE: Biomedical Chromatography (2007), 21(2), 184-189
CODEN: BICHE2; ISSN: 0269-3879
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A liquid chromatog./tandem mass spectrometric method for the quantification of 6-(3-benzoyl-ureido)-hexanoic acid hydroxyamide (EX-2), a novel histone deacetylase (HDAC) inhibitor, in mouse plasma was developed to support inhouse pharmacokinetic (PK) studies in the lead optimization stage. In order to determine the PK parameters for EX-2 in comparison to other HDAC inhibitors such as Suberoylanilide hydroxamic acid (SAHA), PXD-101, and LBH-589, which are currently in different stages of clin. trials, research-grade bio-anal. method validations were carried out for EX-2 and these reference HDAC inhibitors, which were synthesized by inhouse medicinal chemists. The components of validation consisted of specificity, extraction efficiency, signal-response of calibration stds., lower limit of quantification, autosampler stability, and accuracy and precision of quality control samples. The validated LC/MS/MS methods were accurate and precise. The calibration curve ranged from 1 to 1600 ng/mL for all the analytes. The methods developed were used to quantify EX-2 and other HDAC inhibitors in mouse plasma obtained from pharmacokinetic studies. The results suggest that EX-2 has better PK parameters compared with the reference drugs and is a promising drug development candidate.
IT 851365-34-9, EX 2
RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)
(development and validation of HPLC-tandem mass spectrometry assay for (benzoylureido)hexanoic acid hydroxyamide in mouse plasma for pharmacokinetic studies)

Updated Search

stn

RN 851365-34-9 HCAPLUS
CN Benzamide, N-[[[6-(hydroxyamino)-6-oxohexyl]amino]carbonyl]- (CA INDEX NAME)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	19.04	200.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.40	-2.40

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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CAOLD will be discontinued and removed from associated database clusters.

- November 22, 2008 - removed from database clusters
- December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CAplus. To learn more about the options available for transferring saved search queries and answer sets to CA/CAplus, contact your STN Service Center.

=> d his

Updated Search

stn

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1   STRUCTURE UPLOADED
L2   0 S L1
L3   14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4   3 S L3
L5   1 S L4 AND LIM, Z?/AU
L6   2 S L4 NOT L5
L7   0 S L6 AND WANG, H?/AU
L8   0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008

=> s l3
L9   0 L3

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
FULL ESTIMATED COST   0.46   200.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                       ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -2.40

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
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COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\sdfaeat.str

Updated Search

stn

L10 STRUCTURE UPLOADED

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=> s l10
SAMPLE SEARCH INITIATED 00:38:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      337 TO ITERATE

100.0% PROCESSED      337 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:         5639 TO     7841
PROJECTED ANSWERS:               3 TO      163

L11           3 SEA SSS SAM L10

=> s l10 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:38:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     6846 TO ITERATE

100.0% PROCESSED     6846 ITERATIONS                               66 ANSWERS
SEARCH TIME: 00.00.01

L12          66 SEA SSS FUL L10

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1               STRUCTURE UPLOADED
L2             0 S L1
L3            14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
L8             0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9             0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10              STRUCTURE UPLOADED
L11            3 S L10
L12           66 S L10 FULL

=> s l12 not l3
L13          66 L12 NOT L3

=> file hcaplus
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Updated Search

stn

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	180.66	381.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.40

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l13
L14 1 L13

=> d l14, ibib abs fhitstr, 1

L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395258 HCAPLUS
DOCUMENT NUMBER: 142:446921
TITLE: A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors
INVENTOR(S): Lim, Ze-Yi; Wang, Haishan; Zhou, Yan
PATENT ASSIGNEE(S): Sbio Pte. Ltd., Singapore
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

Updated Search

stn

WO 2005040101	A1	20050506	WO 2004-SG353		20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
JP 2007509930	T	20070419	JP 2006-537946		20041026
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US 20080070954	A1	20080320	US 2007-577462		20070927
PRIORITY APPLN. INFO.:			US 2003-514013P	P	20031027
			WO 2004-SG353	W	20041026

OTHER SOURCE(S): CASREACT 142:446921; MARPAT 142:446921

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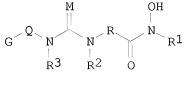

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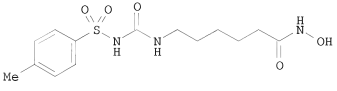


II

AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

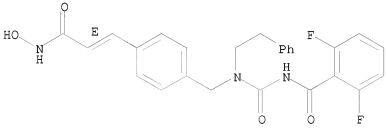
IT 1044042-89-8

Updated Search

stn

RL: PRPH (Prophetic)
(A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors)
RN 1044042-89-8 HCAPLUS
CN Benzamide, 2,6-difluoro-N-[[[[4-[(1E)-3-(hydroxyamino)-3-oxo-1-propen-1-yl]phenyl]methyl](2-phenylethyl)amino]carbonyl]- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	8.14	389.63
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.80	-3.20

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAOLD will be discontinued and removed from associated database clusters.

Updated Search

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    . November 22, 2008 - removed from database clusters
    . December 31, 2008 - removed from STN

  Content previously available only in CAOLD is now available
  in CA/CAplus.  To learn more about the options available for
  transferring saved search queries and answer sets to CA/CAplus,
  contact your STN Service Center.

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1             STRUCTURE UPLOADED
L2           0 S L1
L3          14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4           3 S L3
L5           1 S L4 AND LIM, Z?/AU
L6           2 S L4 NOT L5
L7           0 S L6 AND WANG, H?/AU
L8           0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9           0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10            STRUCTURE UPLOADED
L11          3 S L10
L12         66 S L10 FULL
L13         66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14          1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008

=> s l13
L15          0 L13

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.46     390.09

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                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00      -3.20

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\awerat.str

L16   STRUCTURE UPLOADED

=> s l16
SAMPLE SEARCH INITIATED 00:41:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   337 TO ITERATE

100.0% PROCESSED   337 ITERATIONS   3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 5639 TO   7841
PROJECTED ANSWERS: 3 TO   163

L17   3 SEA SSS SAM L16

=> s l16 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:41:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   6851 TO ITERATE

100.0% PROCESSED   6851 ITERATIONS   69 ANSWERS
SEARCH TIME: 00.00.01

L18   69 SEA SSS FUL L16

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008

Updated Search

stn

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L1              STRUCTURE UPLOADED
L2            0 S L1
L3           14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4            3 S L3
L5            1 S L4 AND LIM, Z?/AU
L6            2 S L4 NOT L5
L7            0 S L6 AND WANG, H?/AU
L8            0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9            0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10             STRUCTURE UPLOADED
L11           3 S L10
L12          66 S L10 FULL
L13          66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14           1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15           0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16             STRUCTURE UPLOADED
L17           3 S L16
L18          69 S L16 FULL

=> s l18 not l3
L19         69 L18 NOT L3

=> s l19 not l13
L20          3 L19 NOT L13

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
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CA SUBSCRIBER PRICE                                     0.00      -3.20

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
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Updated Search

stn

FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l20
L21 1 L20

=> d l21, ibib abs fhitstr, 1

L21 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:395258 HCAPLUS
DOCUMENT NUMBER: 142:446921
TITLE: A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors
INVENTOR(S): Lim, Ze-Yi; Wang, Haishan; Zhou, Yan
PATENT ASSIGNEE(S): Sbio Pte. Ltd., Singapore
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005040101	A1	20050506	WO 2004-SG353	20041026
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004284030	A1	20050506	AU 2004-284030	20041026
CA 2543570	A1	20050506	CA 2004-2543570	20041026
EP 1685094	A1	20060802	EP 2004-775672	20041026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

JP 2007509930	T	20070419	JP 2006-537946		20041026
MX 2006PA04735	A	20061214	MX 2006-PA4735		20060427
US 20080070954	A1	20080320	US 2007-577462		20070927
PRIORITY APPLN. INFO.:			US 2003-514013P	P	20031027
			WO 2004-SG353	W	20041026

OTHER SOURCE(S): CASREACT 142:446921; MARPAT 142:446921

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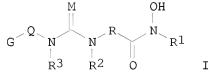

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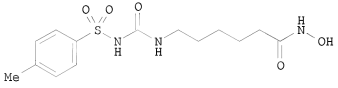


II

AB The invention relates to a preparation of acylurea- and sulfonylurea-connected hydroxamates of formula I [wherein: R is a linking moiety; R1 is H, alkyl, or acyl; M is O, S, NH, NOH, or N(alkyl), etc.; R2 and R3 are independently selected from H, halogen, alkyl, alk(en/yn)yl, or heteroalkyl, etc.; Q is SO2, C(O), or C(S); G is (cyclo)alkyl, (hetero)aryl, or arylalkyl, etc.], useful as HDAC inhibitors. For instance, hexanoic acid derivative II [IC50 (μM): HDAC1 - >100, HDAC8 - 0.79] was prepared from Me 6-aminohexanoate hydrochloride and phenylsulfonyl isocyanate with a yield of 58%.

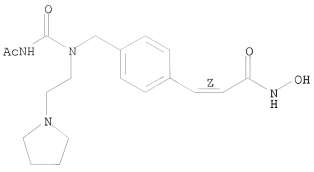
IT 1044042-87-6
RL: PRPH (Prophetic)
(A preparation of acylurea- and sulfonylurea-connected hydroxamates, useful as histone deacetylase (HDAC) inhibitors)

RN 1044042-87-6 HCAPLUS

CN 2-Propenamide, 3-[4-[[[(acetylamino)carbonyl][2-(1-pyrrolidinyl)ethyl]amino]methyl]phenyl]-N-hydroxy-, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

stn



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	8.14	577.97
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.80	-4.00

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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CAOLD will be discontinued and removed from associated database clusters.

- November 22, 2008 - removed from database clusters
- December 31, 2008 - removed from STN

Content previously available only in CAOLD is now available in CA/CAplus. To learn more about the options available for

stn

transferring saved search queries and answer sets to CA/CAplus,
contact your STN Service Center.

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10 STRUCTURE UPLOADED
L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008

=> s l20
L22 0 L20

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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.46 578.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

Updated Search

stn

CA SUBSCRIBER PRICE 0.00 -4.00

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\qqtqt.str

L23 STRUCTURE UPLOADED

=> s l23
SAMPLE SEARCH INITIATED 00:44:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 337 TO ITERATE

100.0% PROCESSED 337 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5639 TO 7841
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

=> s l23 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED - 6851 TO ITERATE

100.0% PROCESSED 6851 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

Updated Search

stn

L25 18 SEA SSS FUL L23

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
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L11 3 S L10
L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21 1 S L20

FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22 0 S L20

FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23 STRUCTURE UPLOADED
L24 0 S L23
L25 18 S L23 FULL

=> s l25 not l13
L26 18 L25 NOT L13

=> s l25 not l3
L27 18 L25 NOT L3

Updated Search

stn

=> s l27 not l18
L28 18 L27 NOT L18

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 180.20 758.63

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -4.00

FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l28
L29 1 L28

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
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L2 0 S L1
L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5

stn

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L7            0 S L6 AND WANG, H?/AU
L8            0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9            0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10             STRUCTURE UPLOADED
L11           3 S L10
L12          66 S L10 FULL
L13          66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14           1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15           0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16             STRUCTURE UPLOADED
L17           3 S L16
L18          69 S L16 FULL
L19          69 S L18 NOT L3
L20           3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21           1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23             STRUCTURE UPLOADED
L24           0 S L23
L25          18 S L23 FULL
L26          18 S L25 NOT L13
L27          18 S L25 NOT L3
L28          18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29           1 S L28

=> s l29  not l21
L30           0 L29 NOT L21

=> file reg
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                                                  ENTRY    SESSION
FULL ESTIMATED COST                                2.69     761.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                  ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -4.00

FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
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Updated Search

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stn


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STRUCTURE FILE UPDATES:   24 OCT 2008  HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES:  24 OCT 2008  HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\fdafagt.str

L31     STRUCTURE UPLOADED

=> s l31
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SAMPLE SCREEN SEARCH COMPLETED -       65 TO ITERATE

100.0% PROCESSED       65 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          817 TO     1783
PROJECTED ANSWERS:               1 TO       80

L32           1 SEA SSS SAM L31

=> s l31 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED -     1581 TO ITERATE

100.0% PROCESSED     1581 ITERATIONS                              23 ANSWERS
SEARCH TIME: 00.00.01

L33          23 SEA SSS FUL L31

=> d his



Updated Search
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stn

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L1                STRUCTURE UPLOADED
L2             0 S L1
L3            14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
L8             0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9             0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10               STRUCTURE UPLOADED
L11            3 S L10
L12           66 S L10 FULL
L13           66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14            1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15            0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16               STRUCTURE UPLOADED
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L18           69 S L16 FULL
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L20            3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21            1 S L20

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L22            0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23               STRUCTURE UPLOADED
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L28           18 S L27 NOT L18

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     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31               STRUCTURE UPLOADED
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Updated Search

stn

L32 1 S L31
L33 23 S L31 FULL

=> s l33 not l13
L34 23 L33 NOT L13

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 179.74 941.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -4.00

FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l34
L35 12 L34

=> d his

(FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1 STRUCTURE UPLOADED
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L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3

stn

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L5            1 S L4 AND LIM, Z?/AU
L6            2 S L4 NOT L5
L7            0 S L6 AND WANG, H?/AU
L8            0 S L6 AND ZHOU, Y?/AU

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L9            0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10             STRUCTURE UPLOADED
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L12          66 S L10 FULL
L13          66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14           1 S L13

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L15           0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16             STRUCTURE UPLOADED
L17           3 S L16
L18          69 S L16 FULL
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L20           3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21           1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23             STRUCTURE UPLOADED
L24           0 S L23
L25          18 S L23 FULL
L26          18 S L25 NOT L13
L27          18 S L25 NOT L3
L28          18 S L27 NOT L18

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L30           0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31             STRUCTURE UPLOADED
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L34          23 S L33 NOT L13

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=> s l35 not l14
L36          11 L35 NOT L14
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Updated Search

stn

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L37           9 L36 NOT L4

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L38           0 L37 AND LIM, Z?/AU

=> s l37 and wang, h?/au
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L40           0 L37 AND ZHOU, Y?/AU

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L37  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:411563  HCAPLUS
DOCUMENT NUMBER:          140:391128
TITLE:                    Preparation of β-aminohydroxamic acids as peptide
                          deformylase (PDF) inhibitors and their medical use
INVENTOR(S):              Takayama, Wataru; Shirasaki, Masahisa; Inoue, Atsushi
PATENT ASSIGNEE(S):       Senju Pharmaceutical Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 44 pp.
                          CODEN: JKXXAF
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     --------------      ----   --------    -------------------    --------
     JP 2004143053        A     20040520    JP 2002-307534         20021022
PRIORITY APPLN. INFO.:                      JP 2002-307534         20021022
OTHER SOURCE(S):          MARPAT 140:391128
AB   R2LG1NHCHR1CH2CONHOH [R1 = C1-5 linear or branched alkyl; R2 =
     (un)substituted aromatic hydrocarbyl, (un)substituted heterocyclyl; G1 = CO,
     SO2; L = G2NH, (CH2)n, CONR4CHR3, etc.; G2 = CO, SO2, bond; n = 0, 1; R3,
     R4 = H, C4-6 alkyl, R3R4 may be bonded to form C3-7 alkylene] or their
     salts, useful for inhibition of drug-resistant bacteria, are prepared  Thus,
     amidation of (3S)-3-aminoheptanoic acid benzyloxyamide HCl salt with
     2-naphthoyl chloride and hydrogenation of the product gave
     (1S)-naphthalene-2-carboxylic acid
     [1-(hydroxycarbamoylmethyl)pentyl]amide, which inhibited Ni-PDF from
     Escherichia coli with IC50 value of 4.656 μM.
IT   688002-83-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of β-aminohydroxamic acids as peptide deformylase
        inhibitors and antibacterial agents)
RN   688002-83-7  HCAPLUS
CN   Benzamide, N-[[[(1S)-1-[2-(hydroxyamino)-2-oxoethyl]pentyl]amino]carbonyl]-
       (CA INDEX NAME)
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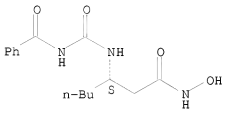
Updated Search

stn

Absolute stereochemistry.



L37 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:381037 HCAPLUS
DOCUMENT NUMBER: 135:133815
TITLE: Protease Inhibitors: Synthesis of a Series of Bacterial Collagenase Inhibitors of the Sulfonyl Amino Acyl Hydroxamate Type
AUTHOR(S): Clare, Brian W.; Scozzafava, Andrea; Supuran, Claudiu T.
CORPORATE SOURCE: Department of Chemistry, The University of Western Australia, 6009, Australia
SOURCE: Journal of Medicinal Chemistry (2001), 44(13), 2253-2258
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:133815

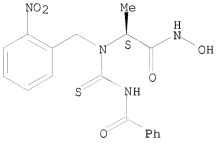
AB A series of sulfonyl amino acyl hydroxamates incorporating alkyl/arylsulfonyl-N-2-nitrobenzyl-L-alanine was prepared Related compds. were obtained by reaction of N-2-nitrobenzyl-L-Ala with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the conversion of the COOH into the CONHOH moiety. The new compds. were assayed as inhibitors of the Clostridium histolyticum collagenase (ChC), a bacterial protease involved in the degradation of extracellular matrix. Many of the obtained hydroxamates proved to be effective bacterial collagenase inhibitors, the main contributor to activity being the substitution pattern at the sulfonamido moiety. The best ChC inhibitors were those containing pentafluorophenylsulfonyl and 3- and 4-protected-aminophenylsulfonyl P1' groups among others, with affinities in the low nanomolar range. This study also proves that the 2-nitrobenzyl- moiety, similarly to the 4-nitrobenyl one previously investigated is an efficient P2' anchoring moiety for obtaining potent bacterial collagenase inhibitors.

IT 351527-61-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of a series of bacterial collagenase inhibitors of the sulfonyl amino acyl hydroxamate type)

RN 351527-61-2 HCAPLUS
CN Benzamide, N-[[[(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl][(2-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)

Updated Search

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:453771 HCAPLUS
DOCUMENT NUMBER: 133:234316
TITLE: Protease inhibitors. Part 12. Synthesis of potent matrix metalloproteinase and bacterial collagenase inhibitors incorporating sulfonylated N-4-nitrobenzyl-β-alanine hydroxamate moieties
AUTHOR(S): Scozzafava, A.; Ilies, M. A.; Manole, G.; Supuran, C. T.
CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, I-50121, Italy
SOURCE: European Journal of Pharmaceutical Sciences (2000), 11(1), 69-79
CODEN: EPSCED; ISSN: 0928-0987
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

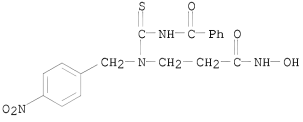
AB N-4-Nitrobenzyl-β-alanine was reacted with alkyl/arylsulfonyl halides, followed by conversion of the COOH to the CONHOH group. Structurally related compds. were obtained by reaction of N-4-nitrobenzyl-β-alanine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by similar conversion of the COOH into the CONHOH moiety. Another subseries of derivs. was prepared from sulfanilyl- or metanilyl-4-nitrobenzyl-β-alanine by reaction with arylsulfonyl isocyanates, followed by the introduction of the hydroxamate moiety. The new compds. were assayed as inhibitors of four matrix metalloproteinases (MMPs), MMP-1, MMP-2, MMP-8 and MMP-9, and of the Clostridium histolyticum collagenase (ChC). Some of the prepared hydroxamate derivs. proved to be very effective collagenase/gelatinase inhibitors, depending on the substitution pattern at the sulfonamido moiety. Substitutions leading to the best inhibitors of MMP-1, a short-pocket enzyme, were those involving pentafluorophenylsulfonyl or 3-trifluoromethyl-phenylsulfonyl at P1' (KI of 3-5 nM). For MMP-2, MMP-8 and MMP-9 (deep-pocket enzymes), the best inhibitors were those containing perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl-, 3- and 4-carboxy-phenylsulfonyl-, arylsulfonylureido- or arylsulfonylureido-sulfanilyl-/metanilyl moieties at P1'. Bulkier groups

in this position, such as 1- and 2-naphthyl-, substituted-naphthyl or quinoline-8-yl- moieties, among others, led to less effective MMP/ChC inhibitors. The best ChC inhibitors were again those containing pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl P1' groups. This study demonstrates that the 4-nitrobenzyl moiety, investigated here for the first time, is an efficient P2' anchoring moiety, whereas the β-alanyl scaffold can successfully replace the α-amino acyl one, for obtaining potent MMP/ChC inhibitors.

IT 294200-81-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of potent matrix metalloproteinase and bacterial collagenase inhibitors incorporating sulfonylated nitrobenzylalanine hydroxamate moieties)

RN 294200-81-0 HCAPLUS

CN Benzamide, N-[[[3-(hydroxyamino)-3-oxopropyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:368315 HCAPLUS

DOCUMENT NUMBER: 133:177439

TITLE: Protease inhibitors: synthesis of L-alanine hydroxamate sulfonylated derivatives as inhibitors of Clostridium histolyticum collagenase

AUTHOR(S): Supuran, Claudiu T.; Briganti, Fabrizio; Mincione, Giovanna; Scozzafava, Andrea

CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, I-50121, Italy

SOURCE: Journal of Enzyme Inhibition (2000), 15(2), 111-128
CODEN: ENINEG; ISSN: 8755-5093

PUBLISHER: Harwood Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB L-alanine hydroxamate derivs. were obtained by reaction of alkyl/arylsulfonyl halides with L-alanine, followed by treatment with benzyl chloride, and conversion of the COOH moiety to the CONHOH group with hydroxylamine in the presence of carbodiimides. Other derivs. were obtained by reaction of N-benzyl-alanine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by a similar conversion of the COOH to the CONHOH moiety. The obtained compds. were assayed as inhibitors of Clostridium histolyticum collagenase, ChC (EC

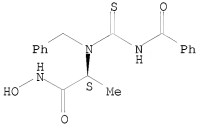
3.4.24.3), a zinc enzyme which degrades triple helical collagen. The hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized derivs., substitution patterns leading to the most potent ChC inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl-, 3- and 4-carboxyphenylsulfonyl-, 3-trifluoromethyl-phenylsulfonyl-, or 1- and 2-naphthylsulfonyl among others. Similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' sites, in order to achieve tight binding to the enzyme.

IT 288266-41-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of L-alanine hydroxamate sulfonylated derivs. as inhibitors of Clostridium histolyticum collagenase)

RN 288266-41-1 HCAPLUS

CN Benzamide, N-[[[(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:261412 HCAPLUS

DOCUMENT NUMBER: 133:53160

TITLE: Protease inhibitors - part 5. Alkyl/arylsulfonyl- and arylsulfonylureido-/arylureido- glycine hydroxamate inhibitors of Clostridium histolyticum collagenase

AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.

CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

SOURCE: European Journal of Medicinal Chemistry (2000), 35(3), 299-307
CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

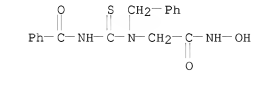
AB Reaction of alkyl/arylsulfonyl halides with glycine afforded a series of derivs. which were first N-benzylated by treatment with benzyl chloride, and then converted to the corresponding hydroxamic acids with

hydroxylamine in the presence of carbodiimide derivs. Other derivs. were obtained by reaction of N-benzyl-glycine with aryl isocyanates, arylsulfonyl isocyanates or benzoyl isothiocyanate, followed by conversion of their COOH group into the CONHOH moiety, as mentioned above. The 90 new compds. reported here were assayed as inhibitors of the Clostridium histolyticum collagenase (EC 3.4.24.3), a zinc enzyme which degrades triple helical regions of native collagen. The prepared hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized hydroxamates, substitution patterns leading to the best inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-carboxyphenylsulfonyl-, 3-trifluoromethyl-phenylsulfonyl or 1- and 2-naphthyl among others. Thus, it seems that similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, Clostridium histolyticum collagenase inhibitors should incorporate hydrophobic moieties at the P1' and P2' sites, whereas the α-carbon substituent may be a small and compact moiety (such as H, for the Gly derivs. reported here). Such compds. might lead to the design of collagenase inhibitor-based drugs useful as anti-cancer, anti-arthritis or anti-bacterial agents for the treatment of corneal keratitis.

IT 276696-17-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(alkyl/arylsulfonyl- and arylsulfonylureido-/arylureido- glycine hydroxamate inhibitors of Clostridium histolyticum collagenase)

RN 276696-17-4 HCAPLUS

CN Benzamide, N-[[[2-(hydroxyamino)-2-oxoethyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:222313 HCAPLUS

DOCUMENT NUMBER: 133:26475

TITLE: Protease Inhibitors: Synthesis of Potent Bacterial Collagenase and Matrix Metalloproteinase Inhibitors Incorporating N-4-Nitrobenzylsulfonylglycine Hydroxamate Moieties

AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.

CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

SOURCE: Journal of Medicinal Chemistry (2000), 43(9), 1858-1865
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of compds. was prepared by reaction of alkyl/arylsulfonyl halides with N-4-nitrobenzylglycine, followed by conversion of the COOH to the CONHOH group, with hydroxylamine in the presence of carbodiimides. Other structurally related compds. were obtained by reaction of N-4-nitrobenzylglycine with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the similar conversion of the COOH into the CONHOH moiety. Another subseries of derivs. was prepared from sulfanilyl- or metanilyl-4-nitrobenzylglycine by reaction with arylsulfonyl isocyanates, followed by conversion of the COOH to the hydroxamate moiety. The new compds. were assayed as inhibitors of four matrix metalloproteinases (MMPs), MMP-1, MMP-2, MMP-8, and MMP-9, and of the Clostridium histolyticum collagenase (ChC). Some of the prepared hydroxamate derivs. proved to be very effective collagenase/gelatinase inhibitors, depending on the substitution pattern at the sulfonamido moiety. Substitutions leading to best inhibitors of MMP-1, a short pocket enzyme, were those involving pentafluorophenylsulfonyl or 3-trifluoromethylphenylsulfonyl moieties at P1' (KI's of 3-5 nM). For MMP-2, MMP-8, and MMP-9 (deep-pocket enzymes), best inhibitors were especially those containing long perfluoroalkylsulfonyl and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl, 3- and 4-protected-aminophenylsulfonyl, 3- and 4-carboxyphenylsulfonyl, arylsulfonylureido, or arylsulfonylureidosulfanilyl/metanilyl moieties, at P1'. Bulkier groups in this position, such as 1- and 2-naphthyl, substituted-naphthyl, or quinolin-8-yl moieties among others, led to less effective MMP/ChC inhibitors. Best ChC inhibitors were again those containing pentafluorophenylsulfonyl or 3- and 4-protected-aminophenylsulfonyl P1' anchoring groups, suggesting that this protease is also a short-pocket wider-neck one (more similar to MMP-1). This study also proves that the 4-nitrobenzyl moiety is an efficient P2' anchoring moiety and that sulfonylureido, ureido, or carboxythioureido substitutions at P1' are also tolerated for obtaining potent sulfonylated amino acid hydroxamate-like MMP/ChC inhibitors.

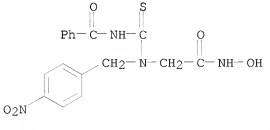
IT 273732-17-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(synthesis of potent bacterial collagenase and matrix metalloproteinase inhibitors incorporating nitrobenzylsulfonylglycine hydroxamate moieties)

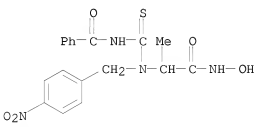
RN 273732-17-5 HCAPLUS

CN Benzamide, N-[[[2-(hydroxyamino)-2-oxoethyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:208763 HCAPLUS
DOCUMENT NUMBER: 132:305057
TITLE: Protease inhibitors: synthesis of Clostridium histolyticum collagenase inhibitors incorporating sulfonyl-L-alanine hydroxamate moieties
AUTHOR(S): Scozzafava, Andrea; Supuran, Claudiu T.
CORPORATE SOURCE: Universita degli Studi, Laboratorio di Chimica Inorganica e Bioinorganica, Florence, 50121, Italy
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(5), 499-502
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of hydroxamates was obtained by the reaction of N-(4-nitrobenzyl)-L-alanine with alkyl/arylsulfonyl halides, followed by conversion of the CO2H group into CONHOH (no data). Structurally related compds. were prepared similarly by using arylsulfonyl isocyanates, aryl isocyanates or arylsulfenyl halides instead of the sulfonyl halides (no data). Many of the new compds. showed nanomolar affinity for the bacterial collagenase isolated from the pathogen Clostridium histolyticum.
IT 265668-57-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Clostridium collagenase inhibitors incorporating sulfonylalanine hydroxamate)
RN 265668-57-3 HCAPLUS
CN Benzamide, N-[[[2-(hydroxyamino)-1-methyl-2-oxoethyl][(4-nitrophenyl)methyl]amino]thioxomethyl]- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:157028 HCAPLUS
DOCUMENT NUMBER: 132:344757
TITLE: Protease inhibitors. Part 8. Synthesis of potent Clostridium histolyticum collagenase inhibitors incorporating sulfonylated L-alanine hydroxamate moieties
AUTHOR(S): Scozzafava, A.; Supuran, C. T.
CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy

SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(3), 637-645
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

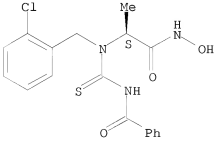
AB A series of hydroxamates was prepared by reaction of alkyl/arylsulfonyl halides with N-2-chlorobenzyl-L-alanine, followed by conversion of the CO2H moiety to the CONHOH group, with NH2OH in the presence of carbodiimides. Other structurally related compds. were obtained by reaction of N-2-chlorobenzyl-L-alanine with aryl isocyanates, arylsulfonyl isocyanates, or benzoyl isothiocyanate, followed by the similar conversion of the CO2H into the CONHOH moiety. The new compds. were assayed as inhibitors of the Clostridium histolyticum collagenase, ChC (EC 3.4.24.3), a bacterial Zn metallo-peptidase which degrades triple helical collagen as well as a large number of synthetic peptides. The prepared hydroxamates proved to be 100-500+ more active collagenase inhibitors than the corresponding carboxylates. Substitution patterns leading to best ChC inhibitors (both for carboxylates as well as for the hydroxamates) were those involving perfluoroalkylsulfonyl- and substituted arylsulfonyl moieties, such as C6F5SO2, protected 3- and 4-aminophenylsulfonyl-, 3-/4-HO2CC6H4SO2, 3-F3CC6H4SO2, as well as 1- and 2-naphthyl-, quinolin-8-yl- or substituted-arylsulfonylamido-carboxyl moieties among others. Similarly to the matrix metalloproteinase (MMP) hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' sites, to achieve tight binding to the enzyme. This study also proves that the 2-chlorobenzyl moiety, is an efficient P2' anchoring moiety for obtaining potent ChC inhibitors.

IT 269747-23-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of Clostridium collagenase inhibitors incorporating sulfonylated alanine hydroxamate)

RN 269747-23-1 HCAPLUS

CN Benzamide, N-[[[(2-chlorophenyl)methyl][(1S)-2-(hydroxyamino)-1-methyl-2-oxoethyl]amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:142412 HCAPLUS

stn

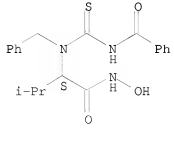
DOCUMENT NUMBER: 132:342787
TITLE: Protease inhibitors. Part 7 Inhibition of Clostridium histolyticum collagenase with sulfonylated derivatives of l-valine hydroxamate
AUTHOR(S): Supuran, C. T.; Scozzafava, A.
CORPORATE SOURCE: Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, I-50121, Italy
SOURCE: European Journal of Pharmaceutical Sciences (2000), 10(1), 67-76
CODEN: EPSCED; ISSN: 0928-0987
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sulfonylated l-valine hydroxamate derivs. were obtained by reaction of alkyl/arylsulfonyl halides with the title amino acid, followed by treatment with benzyl chloride, and conversion of the COOH moiety to the CONHOH group. Other derivs. were obtained by reaction of N-benzyl-l-valine with arylisocyanates, arylsulfonylisocyanates or benzoylisothiocyanate, followed by the similar conversion of the COOH into the CONHOH moiety, with hydroxylamine in the presence of carbodiimides. The obtained compds. were assayed as inhibitors of the Clostridium histolyticum collagenase, ChC (EC 3.4.24.3), a zinc enzyme which degrades triple helical collagen. The hydroxamate derivs. were generally 100-500 times more active than the corresponding carboxylates. In the series of synthesized derivs., substitution patterns leading to best ChC inhibitors were those involving perfluoroalkylsulfonyl- and substituted-arylsulfonyl moieties, such as pentafluorophenylsulfonyl; 3- and 4-protected-aminophenylsulfonyl-; 3- and 4-carboxyphenylsulfonyl-; 3-trifluoromethylphenylsulfonyl; or 1- and 2-naphthyl among others. Similarly to the matrix metalloproteinase hydroxamate inhibitors, ChC inhibitors of the type reported here must incorporate hydrophobic moieties at the P2' and P3' subsites, in order to achieve tight binding to the enzyme. Such compds. might lead to drugs useful in the treatment of corneal bacterial keratitis.

IT 270072-93-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonylated valine hydroxamates as inhibitors of Clostridium histolyticum collagenase)

RN 270072-93-0 HCAPLUS
CN Benzamide, N-[[[(1S)-1-[(hydroxyamino)carbonyl]-2-methylpropyl](phenylmethyl)amino]thioxomethyl]- (CA INDEX NAME)

Absolute stereochemistry.



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REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
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L3 14 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4 3 S L3
L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9 0 S L3

FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10 STRUCTURE UPLOADED
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L12 66 S L10 FULL
L13 66 S L12 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14 1 S L13

FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16 STRUCTURE UPLOADED
L17 3 S L16
L18 69 S L16 FULL
L19 69 S L18 NOT L3
L20 3 S L19 NOT L13

FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
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L23 STRUCTURE UPLOADED
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L27 18 S L25 NOT L3
L28 18 S L27 NOT L18

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L32           1 S L31
L33          23 S L31 FULL
L34          23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
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L36          11 S L35 NOT L14
L37           9 S L36 NOT L4
L38           0 S L37 AND LIM, Z?/AU
L39           0 S L37 AND WANG, H?/AU
L40           0 S L37 AND ZHOU, Y?/AU

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FULL ESTIMATED COST                                75.95    1017.01

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=> s l34
L41 0 L34

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FULL ESTIMATED COST 0.46 1017.47

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L42 STRUCTURE UPLOADED

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SAMPLE SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 608 TO 1472

Updated Search

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stn

PROJECTED ANSWERS:               1 TO       80

L43           1 SEA SSS SAM L42

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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED -     1051 TO ITERATE

100.0% PROCESSED     1051 ITERATIONS                                74 ANSWERS
SEARCH TIME: 00.00.01

L44          74 SEA SSS FUL L42

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DHIS IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d his

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L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
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     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
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Updated Search
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stn

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     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

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Updated Search

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L5            1 S L4 AND LIM, Z?/AU
L6            2 S L4 NOT L5
L7            0 S L6 AND WANG, H?/AU
L8            0 S L6 AND ZHOU, Y?/AU

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L10             STRUCTURE UPLOADED
L11           3 S L10
L12          66 S L10 FULL
L13          66 S L12 NOT L3

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L23             STRUCTURE UPLOADED
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L33          23 S L31 FULL
L34          23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
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stn

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=> s 146 not l13
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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   179.74    1197.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -11.20

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FILE COVERS 1907 - 27 Oct 2008  VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008  (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
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Updated Search

stn

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=> s 147
L48         13 L47

=> d hsi
'HSI' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs
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stn

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

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L3 14 S L1 FULL

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L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

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L12 66 S L10 FULL
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FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
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L15 0 S L13

FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
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L18 69 S L16 FULL
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FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
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stn

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L40             0 S L37 AND ZHOU, Y?/AU

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L44            74 S L42 FULL
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L47            74 S L46 NOT L13

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=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

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L3             14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
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L5              1 S L4 AND LIM, Z?/AU
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Updated Search

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L42               STRUCTURE UPLOADED
L43             1 S L42
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=> d l49, ibib abs hitstr, l-3

L49  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2003:442742  HCAPLUS
DOCUMENT NUMBER:          139:245665
TITLE:                    Novel Inhibitors of Procollagen C-Terminal Proteinase.
                          Part 1: Diamino Acid Hydroxamates
AUTHOR(S):                Delaet, N. G. J.; Robinson, L. A.; Wilson, D. M.;
                          Sullivan, R. W.; Bradley, E. K.; Dankwardt, S. M.;
                          Martin, R. L.; Van Wart, H. E.; Walker, K. A. M.
CORPORATE SOURCE:         CombiChem Inc., San Diego, CA, 92121, USA
SOURCE:                   Bioorganic & Medicinal Chemistry Letters (2003),
                          13(13), 2101-2104
                          CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER:                Elsevier Science B.V.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 139:245665
AB   The parallel synthesis of novel inhibitors of procollagen C-terminal
     proteinase is described.  The synthetic strategy allowed for the facile
     synthesis of a large number of side-chain diversified diamino acid
     hydroxamates, of which the d-diaminopropionic acid derivs. were shown to
     be single digit nanomolar PCP inhibitors.
IT   279255-40-2P
     RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation)
        (solid-phase synthesis and structure-activity relations of diamino acid
        hydroxamates as inhibitors of procollagen C-terminal proteinase)
RN   279255-40-2  HCAPLUS
CN   Propanamide, 2-[(1,3-benzodioxol-5-ylmethyl)[(4-
     methoxyphenyl)sulfonyl]amino]-3-[[[[(4-
     chlorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy-, (2R)-  (CA INDEX
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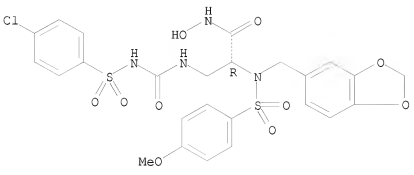
NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

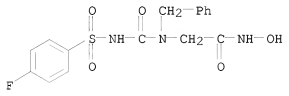
L49 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:311217 HCAPLUS
DOCUMENT NUMBER: 139:245734
TITLE: Protease inhibitors: synthesis of bacterial collagenase and matrix metalloproteinase inhibitors incorporating arylsulfonylureido and 5-dibenzo-suberenyl/suberyl moieties
AUTHOR(S): Ilies, Monica; Banciu, Mircea D.; Scozzafava, Andrea; Ilies, Marc A.; Caproiu, Miron T.; Supuran, Claudiu T.
CORPORATE SOURCE: Polo Scientifico, Laboratorio di Chimica Inorganica e Bioinorganica, Universita degli Studi, Florence, 50019, Italy
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(10), 2227-2239
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245734

AB Novel matrix metalloproteinase (MMP)/bacterial collagenase inhibitors are reported, considering the sulfonylated amino acid hydroxamates as lead mols. A series of compds. was prepared by reaction of arylsulfonyl isocyanates with N-(5H-dibenzo[a,d]cyclohepten-5-yl)- and N-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl) Me glycocolate, resp., followed by the conversion of the COOMe to the carboxylate/hydroxamate moieties. The corresponding derivs. with methylene and ethylene spacers between the polycyclic moiety and the amino acid functionality were also obtained by related synthetic strategies. These new compds. were assayed as inhibitors of MMP-1, MMP-2, MMP-8 and MMP-9, and of the collagenase isolated from Clostridium histolyticum (ChC). Some of the new derivs. reported here proved to be powerful inhibitors of the four MMPs mentioned above and of ChC, with activities in the low nanomolar range for some of the target enzymes, depending on the substitution pattern at the sulfonylureido moiety and on the length of the spacer through which the dibenzosuberenyl/suberyl group is connected with the rest of the mol.

Several of these inhibitors also showed selectivity for the deep pocket enzymes (MMP-2, MMP-8 and MMP-9) over the shallow pocket ones MMP-1 and ChC.

IT 276695-94-4 276695-95-5 276695-96-6
276695-97-7
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of arylsulfonylureido- and dibenzosuberenyl/suberyl-containing compds. as matrix metalloproteinase/bacterial collagenase inhibitors)

RN 276695-94-4 HCAPLUS
CN Acetamide, 2-[[[[(4-fluorophenyl)sulfonyl]amino]carbonyl](phenylmethyl)amino]-N-hydroxy- (CA INDEX NAME)



RN 276695-95-5 HCAPLUS
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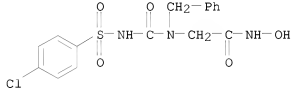

RN 276695-96-6 HCAPLUS
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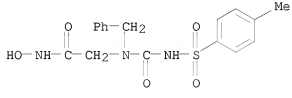

RN 276695-97-7 HCAPLUS
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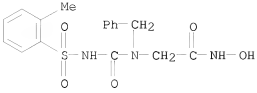

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597570-18-8P 597570-19-9P 597570-20-2P
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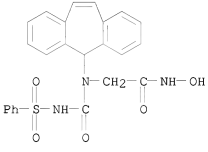
597570-34-8P 597570-37-1P 597570-39-3P
597570-41-7P 597570-43-9P 597570-45-1P
597570-47-3P 597570-49-5P 597570-51-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of arylsulfonylureido- and dibenzosuberenyl/suberyl-containing compds. as matrix metalloproteinase/bacterial collagenase inhibitors)

RN 597570-12-2 HCAPLUS
CN Acetamide, 2-[5H-dibenzo[a,d]cyclohepten-5-yl[[(phenylsulfonyl)amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)



RN 597570-13-3 HCAPLUS
CN Acetamide, 2-[5H-dibenzo[a,d]cyclohepten-5-yl[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy- (CA INDEX NAME)

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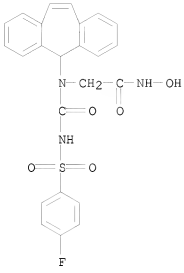

RN 597570-14-4 HCAPLUS
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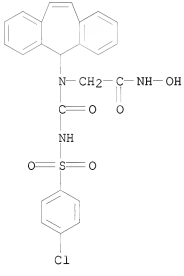

RN 597570-15-5 HCAPLUS
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Updated Search

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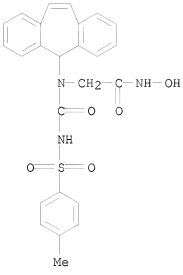

RN 597570-16-6 HCAPLUS
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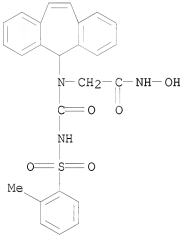

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Updated Search

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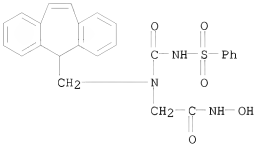

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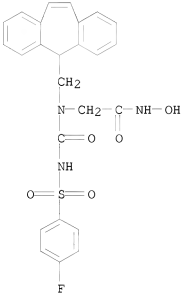

RN 597570-19-9 HCAPLUS
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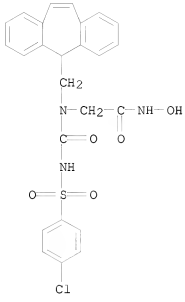
stn



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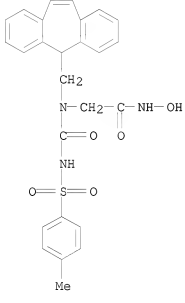

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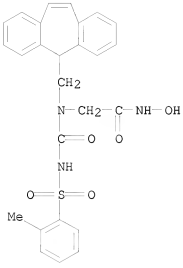
Updated Search



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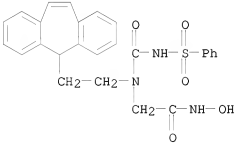

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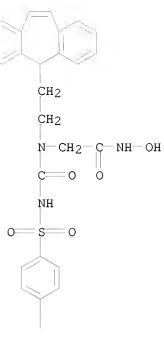
PAGE 1-A



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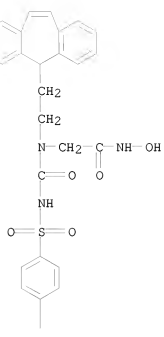

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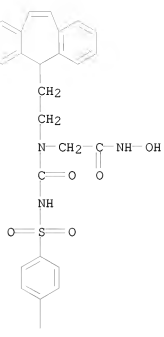
PAGE 1-A



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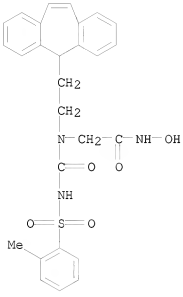

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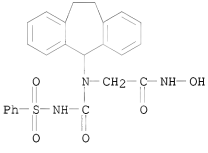

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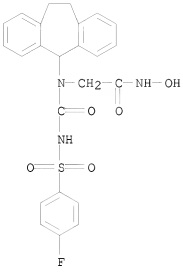
Updated Search

stn



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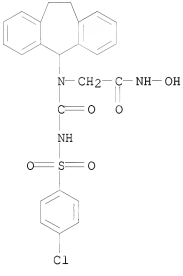

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Updated Search

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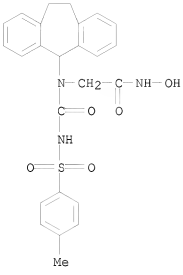

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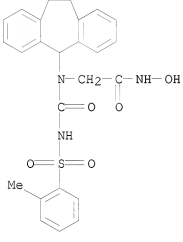

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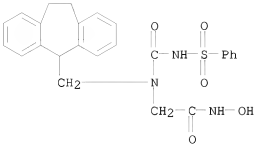
Updated Search



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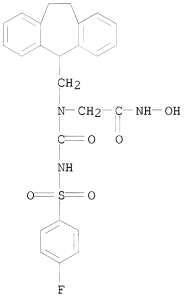

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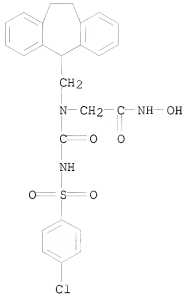

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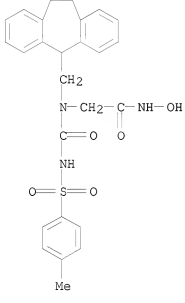

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Updated Search

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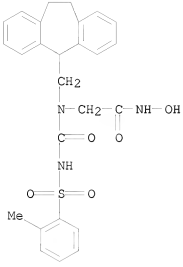

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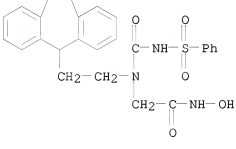

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Updated Search

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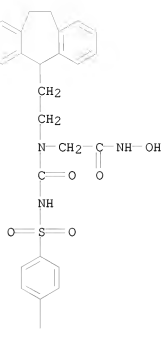
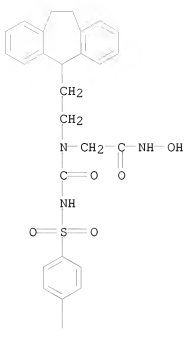


PAGE 2-A

RN 597570-47-3 HCAPLUS
CN Acetamide, 2-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl][2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)ethyl]amino]-N-hydroxy- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

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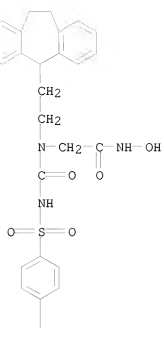
PAGE 1-A



PAGE 2-A

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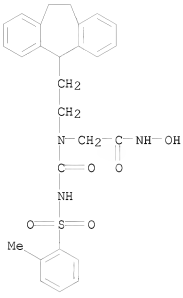

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:441768 HCAPLUS
DOCUMENT NUMBER: 133:74324
TITLE: Preparation of amino acid sulfonamide hydroxamates as inhibitors of procollagen C-proteinase.
INVENTOR(S): Billedeau, Roland Joseph; Broka, Chris Allen; Campbell, Jeffrey Allen; Chen, Jian Jeffrey; Dankwardt, Sharon Marie; Delaet, Nancy; Robinson, Leslie Ann; Walker, Keith Adrian Murray
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000037436	A1	20000629	WO 1999-EP9920	19991214
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2355902	A1	20000629	CA 1999-2355902	19991214
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AT 270271	T	20040715	AT 1999-963530		19991214
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			US 1999-164138P	P	19991108
			WO 1999-EP9920	W	19991214
			US 1999-469660	A3	19991222

OTHER SOURCE(S): MARPAT 133:74324

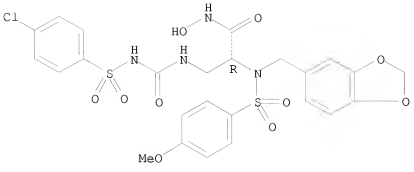
AB HOHNCOCHR1NRSO2Ar2 [R1 = alkyl, haloalkyl, heteroalkyl, cycloalkyl, aryl, aralkyl, aralkenyl, heteroaryl, heteroaralkyl, aminl, aryl, aralkyl, etc.; R = CHR2Ar1, CHR2CH:CHAr1; Ar2 = specified (substituted) Ph, naphthyl; R2 = H, alkyl; with provisos], were prepared Thus, N-hydroxy-2(R)-[(3,4-methylenedioxybenzyl)(4-methoxy-2,3,6-trimethylbenzenesulfonyl)amino]-3-methylbutyramide was prepared by solution phase synthesis from BOC-D-Val-OH. Title compds. inhibited procollagen C-proteinase with IC50 0.01-2 μM.

IT 279255-40-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid sulfonamide hydroxamates as inhibitors of procollagen C-proteinase)

RN 279255-40-2 HCAPLUS

CN Propanamide, 2-[(1,3-benzodioxol-5-ylmethyl)[(4-methoxyphenyl)sulfonyl]amino]-3-[[[[(4-chlorophenyl)sulfonyl]amino]carbonyl]amino]-N-hydroxy-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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CA SUBSCRIBER PRICE	-2.40	-13.60

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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- November 22, 2008 - removed from database clusters
- December 31, 2008 - removed from STN

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L3 14 S L1 FULL

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L5 1 S L4 AND LIM, Z?/AU
L6 2 S L4 NOT L5
L7 0 S L6 AND WANG, H?/AU
L8 0 S L6 AND ZHOU, Y?/AU

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L15 0 S L13

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STRUCTURE FILE UPDATES:   24 OCT 2008  HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES:  24 OCT 2008  HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\asfasry.str

L53     STRUCTURE UPLOADED

=> s l53
SAMPLE SEARCH INITIATED 00:58:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       55 TO ITERATE

100.0% PROCESSED       55 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          656 TO     1544
PROJECTED ANSWERS:               0 TO        0

L54           0 SEA SSS SAM L53

=> s l53 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:58:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1172 TO ITERATE

100.0% PROCESSED     1172 ITERATIONS                              7 ANSWERS
SEARCH TIME: 00.00.01

L55           7 SEA SSS FUL L53

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1             STRUCTURE UPLOADED
L2              0 S L1
L3             14 S L1 FULL



Updated Search
```

stn

```
     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
L8             0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9             0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10              STRUCTURE UPLOADED
L11            3 S L10
L12           66 S L10 FULL
L13           66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14            1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15            0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16              STRUCTURE UPLOADED
L17            3 S L16
L18           69 S L16 FULL
L19           69 S L18 NOT L3
L20            3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21            1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22            0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23              STRUCTURE UPLOADED
L24            0 S L23
L25           18 S L23 FULL
L26           18 S L25 NOT L13
L27           18 S L25 NOT L3
L28           18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29            1 S L28
L30            0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31              STRUCTURE UPLOADED
L32            1 S L31
L33           23 S L31 FULL
L34           23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35           12 S L34
```

Updated Search

stn

```
L36          11 S L35 NOT L14
L37           9 S L36 NOT L4
L38           0 S L37 AND LIM, Z?/AU
L39           0 S L37 AND WANG, H?/AU
L40           0 S L37 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41           0 S L34

     FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42             STRUCTURE UPLOADED
L43           1 S L42
L44          74 S L42 FULL
L45          74 S L44 NOT L34
L46          74 S L45 NOT L19
L47          74 S L46 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48          13 S L47
L49           3 S L48 NOT L35
L50           0 S L49 AND LIM, Z?/AU
L51           0 S L49 AND WANG, H?/AU

     FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52           0 S L47

     FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53             STRUCTURE UPLOADED
L54           0 S L53
L55           7 S L53 FULL

=> s l55 not l47
L56           7 L55 NOT L47

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   179.28    1398.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -13.60

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

```
=> s l56
L57          1 L56

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1               STRUCTURE UPLOADED
L2             0 S L1
L3            14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
L8             0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9             0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10              STRUCTURE UPLOADED
L11            3 S L10
L12           66 S L10 FULL
L13           66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14            1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15            0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16              STRUCTURE UPLOADED
L17            3 S L16
L18           69 S L16 FULL
L19           69 S L18 NOT L3
L20            3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
```

stn

```
L21           1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23             STRUCTURE UPLOADED
L24           0 S L23
L25          18 S L23 FULL
L26          18 S L25 NOT L13
L27          18 S L25 NOT L3
L28          18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29           1 S L28
L30           0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31             STRUCTURE UPLOADED
L32           1 S L31
L33          23 S L31 FULL
L34          23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35          12 S L34
L36          11 S L35 NOT L14
L37           9 S L36 NOT L4
L38           0 S L37 AND LIM, Z?/AU
L39           0 S L37 AND WANG, H?/AU
L40           0 S L37 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41           0 S L34

     FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42             STRUCTURE UPLOADED
L43           1 S L42
L44          74 S L42 FULL
L45          74 S L44 NOT L34
L46          74 S L45 NOT L19
L47          74 S L46 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48          13 S L47
L49           3 S L48 NOT L35
L50           0 S L49 AND LIM, Z?/AU
L51           0 S L49 AND WANG, H?/AU

     FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52           0 S L47

     FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53             STRUCTURE UPLOADED
L54           0 S L53
L55           7 S L53 FULL
L56           7 S L55 NOT L47
```

Updated Search

stn

FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57 1 S L56

=> s l57 not l29
L58 0 L57 NOT L29

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 2.69 1401.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -13.60

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\sadfaerat.str

L59 STRUCTURE UPLOADED

=> s l59
SAMPLE SEARCH INITIATED 01:00:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 52 TO ITERATE

100.0% PROCESSED 52 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

```
stn

PROJECTED ITERATIONS:          608 TO     1472
PROJECTED ANSWERS:               0 TO        0

L60           0 SEA SSS SAM L59

=> s l59 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:00:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1051 TO ITERATE

100.0% PROCESSED     1051 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

L61           2 SEA SSS FUL L59

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1               STRUCTURE UPLOADED
L2             0 S L1
L3            14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
L7             0 S L6 AND WANG, H?/AU
L8             0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9             0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10              STRUCTURE UPLOADED
L11            3 S L10
L12           66 S L10 FULL
L13           66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14            1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15            0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16              STRUCTURE UPLOADED
L17            3 S L16
L18           69 S L16 FULL
L19           69 S L18 NOT L3
L20            3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21            1 S L20
```

stn

```
     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22             0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23               STRUCTURE UPLOADED
L24             0 S L23
L25            18 S L23 FULL
L26            18 S L25 NOT L13
L27            18 S L25 NOT L3
L28            18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29             1 S L28
L30             0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31               STRUCTURE UPLOADED
L32             1 S L31
L33            23 S L31 FULL
L34            23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35            12 S L34
L36            11 S L35 NOT L14
L37             9 S L36 NOT L4
L38             0 S L37 AND LIM, Z?/AU
L39             0 S L37 AND WANG, H?/AU
L40             0 S L37 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41             0 S L34

     FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42               STRUCTURE UPLOADED
L43             1 S L42
L44            74 S L42 FULL
L45            74 S L44 NOT L34
L46            74 S L45 NOT L19
L47            74 S L46 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48            13 S L47
L49             3 S L48 NOT L35
L50             0 S L49 AND LIM, Z?/AU
L51             0 S L49 AND WANG, H?/AU

     FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52             0 S L47

     FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53               STRUCTURE UPLOADED
L54             0 S L53
L55             7 S L53 FULL
L56             7 S L55 NOT L47
```

Updated Search

stn

```
     FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57            1 S L56
L58            0 S L57 NOT L29

     FILE 'REGISTRY' ENTERED AT 00:59:15 ON 27 OCT 2008
L59              STRUCTURE UPLOADED
L60            0 S L59
L61            2 S L59 FULL

=> s l61 not l57
L62            0 L61 NOT L57

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\e-Red
Folder\10524345\araty.str

L63     STRUCTURE UPLOADED

=> s l63
SAMPLE SEARCH INITIATED 01:02:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       65 TO ITERATE

100.0% PROCESSED       65 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          817 TO     1783
PROJECTED ANSWERS:               0 TO        0

L64            0 SEA SSS SAM L63

=> s l63 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 01:02:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1581 TO ITERATE

100.0% PROCESSED     1581 ITERATIONS                                2 ANSWERS
SEARCH TIME: 00.00.01

L65            2 SEA SSS FUL L63

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1               STRUCTURE UPLOADED
L2             0 S L1
L3            14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4             3 S L3
L5             1 S L4 AND LIM, Z?/AU
L6             2 S L4 NOT L5
```

Updated Search

```
L7            0 S L6 AND WANG, H?/AU
L8            0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9            0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10             STRUCTURE UPLOADED
L11           3 S L10
L12          66 S L10 FULL
L13          66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14           1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15           0 S L13

     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16             STRUCTURE UPLOADED
L17           3 S L16
L18          69 S L16 FULL
L19          69 S L18 NOT L3
L20           3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21           1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23             STRUCTURE UPLOADED
L24           0 S L23
L25          18 S L23 FULL
L26          18 S L25 NOT L13
L27          18 S L25 NOT L3
L28          18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29           1 S L28
L30           0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31             STRUCTURE UPLOADED
L32           1 S L31
L33          23 S L31 FULL
L34          23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35          12 S L34
L36          11 S L35 NOT L14
L37           9 S L36 NOT L4
L38           0 S L37 AND LIM, Z?/AU
L39           0 S L37 AND WANG, H?/AU
L40           0 S L37 AND ZHOU, Y?/AU
```

stn

```
     FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41             0 S L34

     FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42               STRUCTURE UPLOADED
L43             1 S L42
L44            74 S L42 FULL
L45            74 S L44 NOT L34
L46            74 S L45 NOT L19
L47            74 S L46 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48            13 S L47
L49             3 S L48 NOT L35
L50             0 S L49 AND LIM, Z?/AU
L51             0 S L49 AND WANG, H?/AU

     FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52             0 S L47

     FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53               STRUCTURE UPLOADED
L54             0 S L53
L55             7 S L53 FULL
L56             7 S L55 NOT L47

     FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57             1 S L56
L58             0 S L57 NOT L29

     FILE 'REGISTRY' ENTERED AT 00:59:15 ON 27 OCT 2008
L59               STRUCTURE UPLOADED
L60             0 S L59
L61             2 S L59 FULL
L62             0 S L61 NOT L57
L63               STRUCTURE UPLOADED
L64             0 S L63
L65             2 S L63 FULL

=> s l65 not l56
L66             2 L65 NOT L56

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    358.10    1759.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00     -13.60

FILE 'HCAPLUS' ENTERED AT 01:02:29 ON 27 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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```

Updated Search

stn

FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l65
L67   1 L65

=> d his

     (FILE 'HOME' ENTERED AT 00:30:07 ON 27 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 00:30:14 ON 27 OCT 2008
L1   STRUCTURE UPLOADED
L2   0 S L1
L3   14 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 00:34:08 ON 27 OCT 2008
L4   3 S L3
L5   1 S L4 AND LIM, Z?/AU
L6   2 S L4 NOT L5
L7   0 S L6 AND WANG, H?/AU
L8   0 S L6 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:34:58 ON 27 OCT 2008
L9   0 S L3

     FILE 'REGISTRY' ENTERED AT 00:35:09 ON 27 OCT 2008
L10   STRUCTURE UPLOADED
L11   3 S L10
L12   66 S L10 FULL
L13   66 S L12 NOT L3

     FILE 'HCAPLUS' ENTERED AT 00:38:27 ON 27 OCT 2008
L14   1 S L13

     FILE 'CAOLD' ENTERED AT 00:38:49 ON 27 OCT 2008
L15   0 S L13

Updated Search

stn

```
     FILE 'REGISTRY' ENTERED AT 00:38:55 ON 27 OCT 2008
L16             STRUCTURE UPLOADED
L17           3 S L16
L18          69 S L16 FULL
L19          69 S L18 NOT L3
L20           3 S L19 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:41:23 ON 27 OCT 2008
L21           1 S L20

     FILE 'CAOLD' ENTERED AT 00:41:37 ON 27 OCT 2008
L22           0 S L20

     FILE 'REGISTRY' ENTERED AT 00:41:44 ON 27 OCT 2008
L23             STRUCTURE UPLOADED
L24           0 S L23
L25          18 S L23 FULL
L26          18 S L25 NOT L13
L27          18 S L25 NOT L3
L28          18 S L27 NOT L18

     FILE 'HCAPLUS' ENTERED AT 00:45:00 ON 27 OCT 2008
L29           1 S L28
L30           0 S L29  NOT L21

     FILE 'REGISTRY' ENTERED AT 00:45:12 ON 27 OCT 2008
L31             STRUCTURE UPLOADED
L32           1 S L31
L33          23 S L31 FULL
L34          23 S L33 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:47:19 ON 27 OCT 2008
L35          12 S L34
L36          11 S L35 NOT L14
L37           9 S L36 NOT L4
L38           0 S L37 AND LIM, Z?/AU
L39           0 S L37 AND WANG, H?/AU
L40           0 S L37 AND ZHOU, Y?/AU

     FILE 'CAOLD' ENTERED AT 00:53:34 ON 27 OCT 2008
L41           0 S L34

     FILE 'REGISTRY' ENTERED AT 00:53:39 ON 27 OCT 2008
L42             STRUCTURE UPLOADED
L43           1 S L42
L44          74 S L42 FULL
L45          74 S L44 NOT L34
L46          74 S L45 NOT L19
L47          74 S L46 NOT L13

     FILE 'HCAPLUS' ENTERED AT 00:55:54 ON 27 OCT 2008
L48          13 S L47
L49           3 S L48 NOT L35
L50           0 S L49 AND LIM, Z?/AU
L51           0 S L49 AND WANG, H?/AU
```

Updated Search

stn

```
     FILE 'CAOLD' ENTERED AT 00:57:13 ON 27 OCT 2008
L52             0 S L47

     FILE 'REGISTRY' ENTERED AT 00:57:20 ON 27 OCT 2008
L53               STRUCTURE UPLOADED
L54             0 S L53
L55             7 S L53 FULL
L56             7 S L55 NOT L47

     FILE 'HCAPLUS' ENTERED AT 00:59:01 ON 27 OCT 2008
L57             1 S L56
L58             0 S L57 NOT L29

     FILE 'REGISTRY' ENTERED AT 00:59:15 ON 27 OCT 2008
L59               STRUCTURE UPLOADED
L60             0 S L59
L61             2 S L59 FULL
L62             0 S L61 NOT L57
L63               STRUCTURE UPLOADED
L64             0 S L63
L65             2 S L63 FULL
L66             2 S L65 NOT L56

     FILE 'HCAPLUS' ENTERED AT 01:02:29 ON 27 OCT 2008
L67             1 S L65

=> s l67 not l57
L68             0 L67 NOT L57
```

Updated Search